The Rayleigh-Taylor Instability via Direct Simulation Monte Carlo

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The Rayleigh-Taylor (RT) instability occurs whenever a high-density fluid rests on top of a low-density fluid in the presence of a gravitational field g. This arrangement is an unstable equilibrium, and the two fluids will subsequently mix in a process that is a classic example of turbulent mixing. For this reason, the RT instability has been widely investigated over the years, both experimentally and theoretically, starting with Rayleigh in 1883. It has many applications in the study of supernovae, geophysical phenomena such as salt domes or volcanic islands, inertial confinement fusion, and in many other areas.

In recent years the RT instability has been studied via computer simulation. While most simulations have been done using continuum methods, there have also been efforts to perform atomistically based RT simulations that take into account the effects of small-scale thermal fluctuations. This avoids the symmetry or artificiality present in the initial conditions of most continuum RT schemes. Previous work along these lines has involved the use of molecular dynamics (MD) to model the RT instability using on the order of 100,000,000 particles [1]. Due to the computationally intensive nature of MD, systems studied by this method are necessarily restricted to very small length and time scales, which has prompted use of the term "nanohydrodynamics" to refer to these types of calculations. Furthermore, in order to see significant mixing on accessible time scales, it becomes necessary to use a very large value of the gravitational acceleration g, i.e., approximately 10 billion multiples of earth's gravity in real units.

In the present work, an alternative particle-based scheme known as Direct Simulation Monte Carlo (DSMC) has been applied to the RT instability. Invented by Bird in the late 1960s, DSMC is a Monte Carlo method in which particle collisions are simulated stochastically rather than being calculated explicitly [2]. In addition, DSMC allows the use of a much larger time step. These, and other, factors result in a significant computational speedup when compared to traditional MD. For example, whereas the previous MD work required approximately 250 hours on 1600 CPUs of the ASC Q computer system at Los Alamos, a preliminary DSMC run of about 60,000,000 particles required only 256 processors and less than 12 hours to reach a more advanced point in the development of the flow. In terms of CPU-seconds per particle, this amounts to an increase in speed by a factor of at least 50, even when variations in simulation parameters are taken into account.

Fig. 1.
The local number fraction of heavy particles in the well-developed flow. This is given by n_h/n, where nh is the number density of heavy particles, and n is the total number density. Red corresponds to $n_h/n=1$, and blue corresponds to $n_h/n=0$.

The DSMC run described above was performed using the Scalable Parallel Short-range MD (SPaSM) code [3], and involved the use of 14,370,860 heavy particles of mass $m_h=5$ and 43,214,549

light particles of mass m_l=1 in the presence of a gravitational field g=0.00025. The system was run in thin slab geometry with periodic boundary conditions in the horizontal directions and specular boundary conditions at the top and bottom. A typical image from the well-developed stage of the flow is shown in Fig. 1. We see that the light fluid moves upward into the heavy fluid in large extrusions known as "bubbles." At the same time, the heavy fluid penetrates the lighter fluid in longer, thinner features known as "spikes."

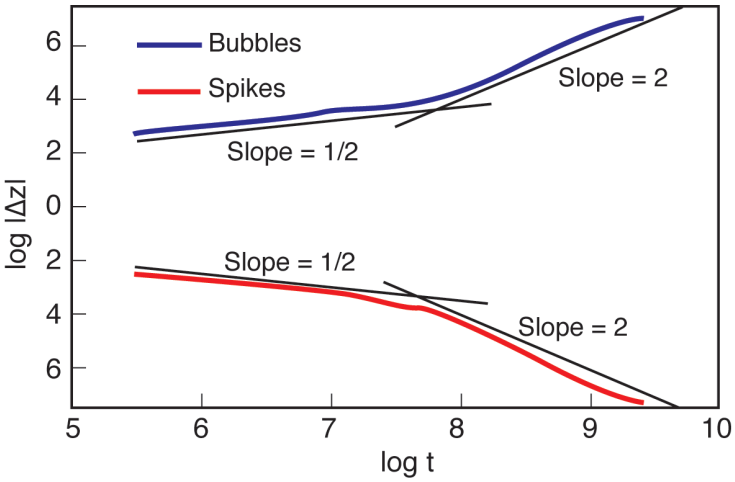

Fig. 2.
A log-log plot of the penetration depth Δz as a function of time for both bubbles and spikes.

It has been found in experiment and predicted by Young that in the turbulent regime the penetration depth of the bubbles and spikes will grow as αAgt^2, where $A=(m_h-m_l)/(m_h+m_l)$ is the Atwood number at the interface. The growth of the bubbles and spikes is shown in Fig. 2. As predicted, the penetration depth grows approximately quadratically in t, with α values of about 0.05 and 0.06 for bubbles and spikes, respectively. These values are consistent with the values obtained in experiment, as well as in previous continuum and MD simulations.

Another feature visible in Fig. 2 is the fact that the penetration depth scales as the square root of t for short times. This is a reflection of the fact that, for small t, the dynamics of the interface are dominated by thermal fluctuations due to the random initial atomic coordinates. It is a diffusive effect, which results from the random walks of individual particles. It should be noted that this physical behavior is not accessible in most standard continuum schemes.

Much of the utility of applying DSMC, rather than MD, to the RT instability comes from the fact that the greater speed of DSMC means that larger systems may be considered for longer periods of time, and using a smaller value of g. This allows the simulation of systems that transcend the nanohydrodynamic regime. For example, if we assume that the preliminary run described above has argon as the lighter species, then its width corresponds to about 3 microns in real units. This makes a DSMC simulation of the RT instability better suited for comparison with more traditional continuum schemes, and also with experiments.

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